LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111422\
Data File : VX032799.D
Acq On : 14 Nov 2022 16:59
Operator : JC/MD
Sample : N5572-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31915

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Title : SW846 8260

Signal : TIC: VX032799.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.459	57	61	65	rBV	11450	14887	1.40%	0.275%
2	2.294	192	198	206	rBV	9499	14960	1.41%	0.276%
3	2.385	206	213	225	rBV	85922	168378	15.84%	3.111%
4	2.709	260	266	274	rVB	7728	14662	1.38%	0.271%
5	3.330	358	368	377	rBV	7979	18559	1.75%	0.343%
6	4.227	505	515	538	rBV	245723	664676	62.53%	12.282%
7	4.556	560	569	587	rVB	88818	261484	24.60%	4.832%
8	5.385	693	705	721	rBV	63224	185400	17.44%	3.426%
9	5.556	721	733	748	rVB	99789	284151	26.73%	5.251%
10	5.958	788	799	820	rBV	66809	179404	16.88%	3.315%
11	6.763	920	931	943	rBV	152805	366347	34.47%	6.769%
12	7.244	1002	1010	1026	rBV2	11979	42080	3.96%	0.778%
13	7.574	1053	1064	1074	rBV	45403	89968	8.46%	1.662%
14	8.573	1221	1228	1234	rBV	24344	39076	3.68%	0.722%
15	8.647	1234	1240	1248	rVV	330256	513038	48.27%	9.480%
16	9.531	1379	1385	1391	rBV3	6881	14147	1.33%	0.261%
17	10.055	1465	1471	1481	rVB	323674	437999	41.21%	8.093%
18	10.158	1483	1488	1500	rVV2	8681	12479	1.17%	0.231%
19	10.683	1570	1574	1580	rVB	15204	18080	1.70%	0.334%
20	10.756	1580	1586	1593	rBV	24390	36762	3.46%	0.679%
21	11.079	1634	1639	1645	rBV	304622	392893	36.96%	7.260%
22	11.420	1691	1695	1702	rBV	16239	21002	1.98%	0.388%
23	11.573	1715	1720	1723	rBV2	11585	15833	1.49%	0.293%
24	11.603	1723	1725	1733	rVB2	10145	13431	1.26%	0.248%
25	11.865	1765	1768	1777	rVB2	9876	21232	2.00%	0.392%
26	12.024	1789	1794	1802	rVB	352405	443610	41.74%	8.197%
27	12.219	1821	1826	1837	rBV	817134	1062890	100.00%	19.640%
28	12.304	1837	1840	1854	rVB3	26956	53266	5.01%	0.984%
29	12.567	1877	1883	1893	rVB6	4722	11163	1.05%	0.206%

Sum of corrected areas: 5411857

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ClientSampleId :
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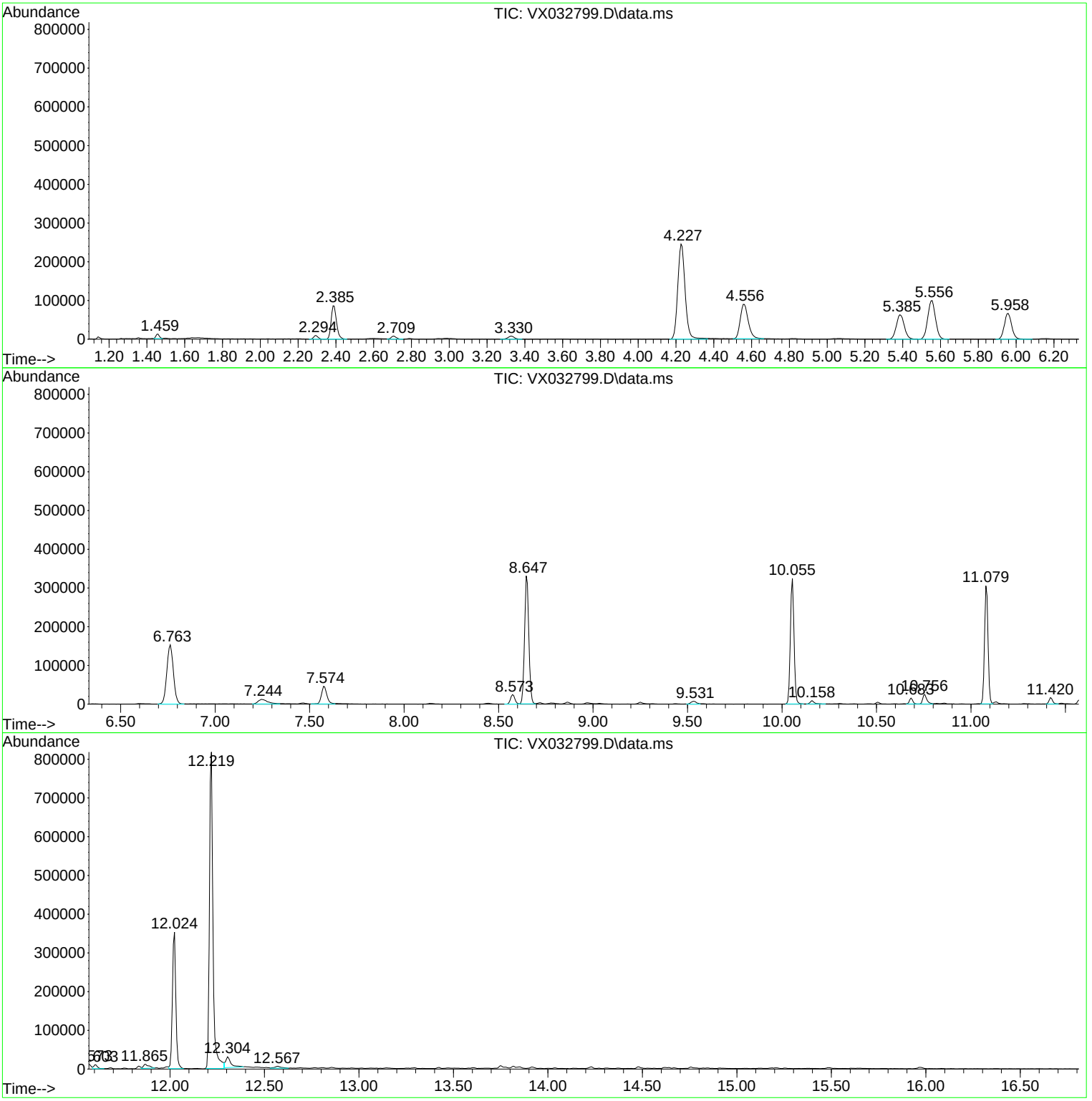
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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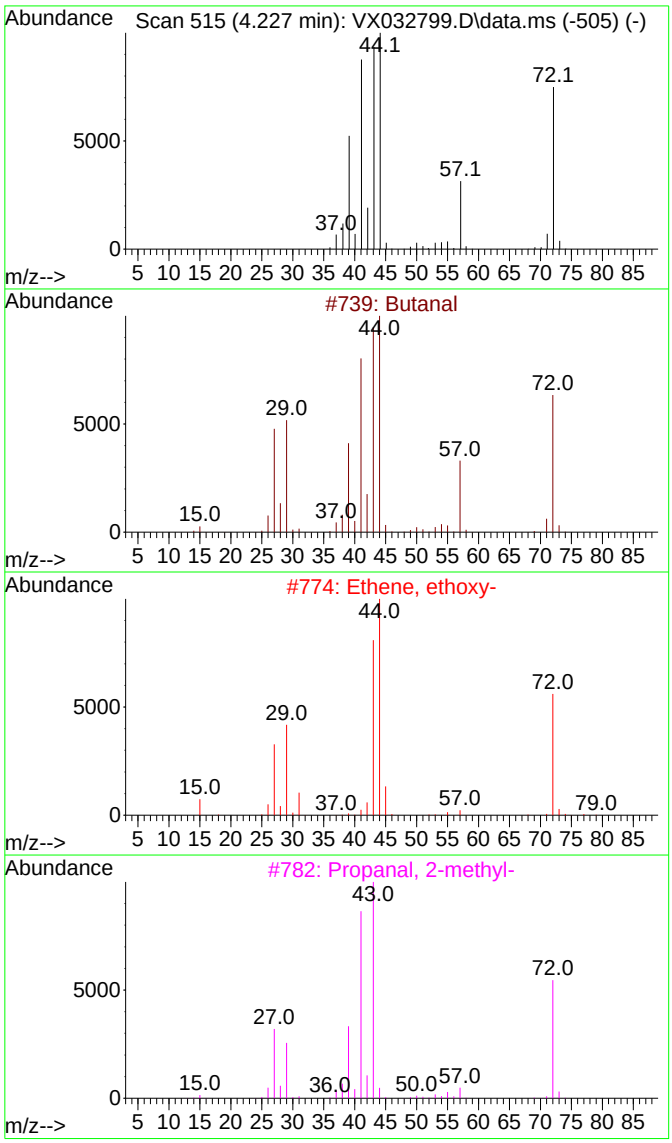
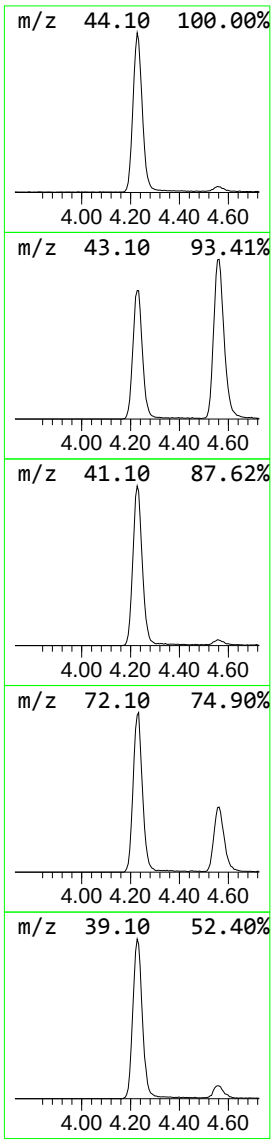
Peak Number 1 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.227	116.96 ug/l	664676	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	94
2	Ethene, ethoxy-	72	C4H8O	000109-92-2	52
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	49
4	Propane	44	C3H8	000074-98-6	47
5	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	37





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TIC Library : C:\Database\NIST20.L
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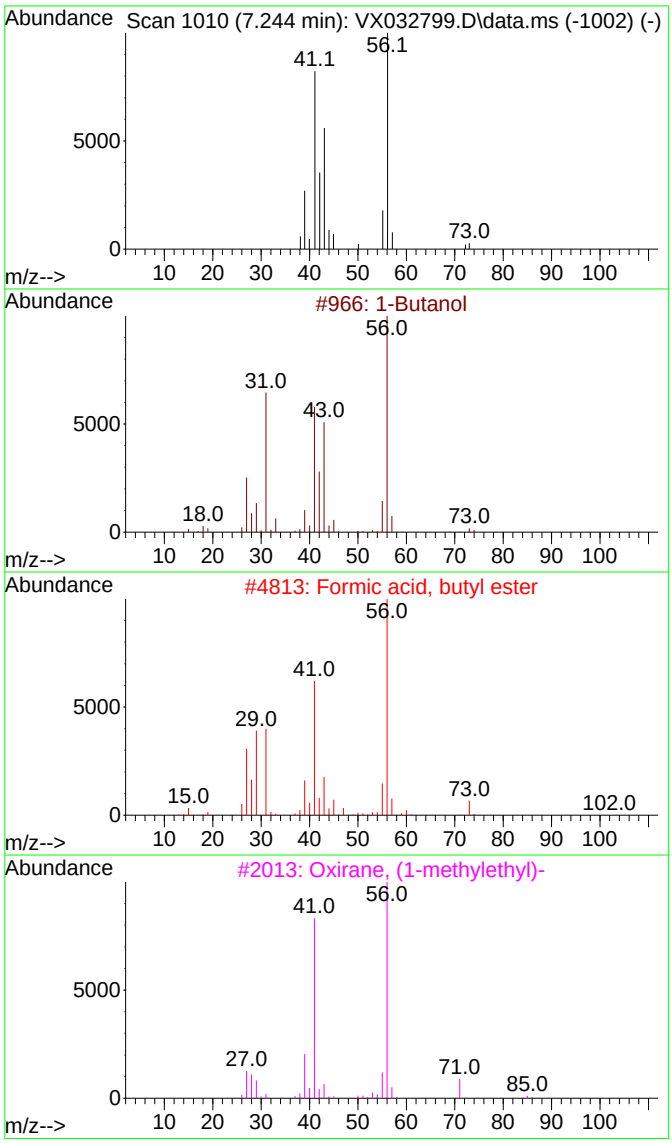
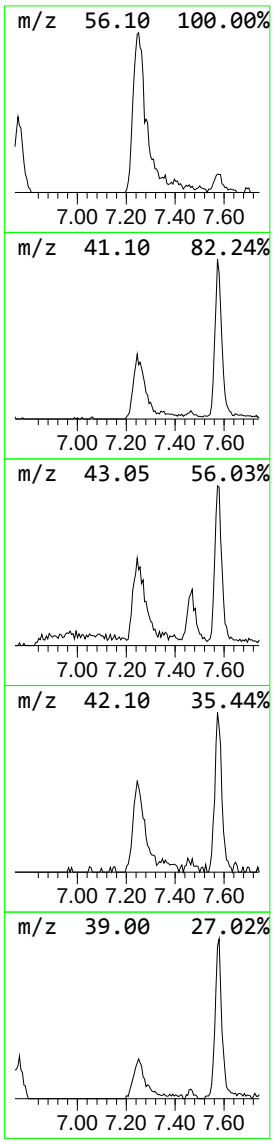
Peak Number 2 1-Butanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.244	5.74 ug/l	42080	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	83
2	Formic acid, butyl ester	102	C5H10O2	000592-84-7	9
3	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	9
4	1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	9
5	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	9





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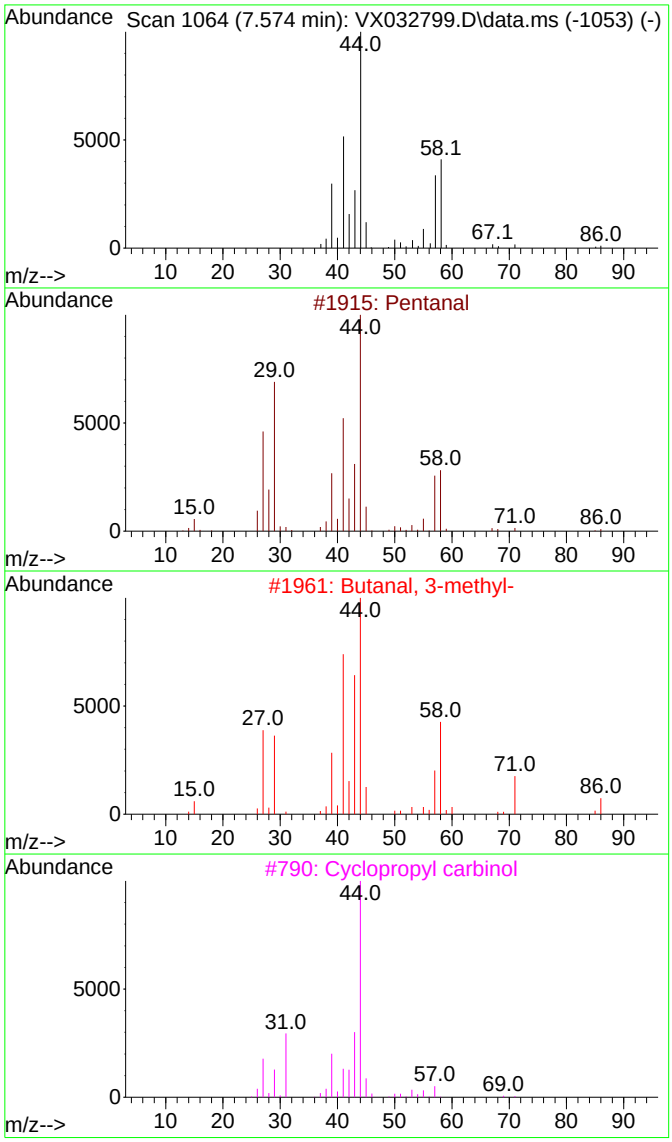
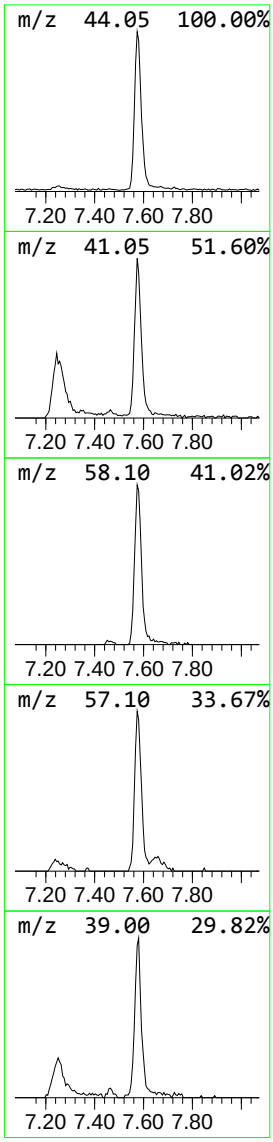
Peak Number 3 Pentanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.574	12.28 ug/l	89968	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal	86	C5H10O	000110-62-3	90
2	Butanal, 3-methyl-	86	C5H10O	000590-86-3	64
3	Cyclopropyl carbinol	72	C4H8O	002516-33-8	40
4	(2-Cyclohexylpropyl)(methyl)amine	155	C10H21N	000532-52-5	9
5	Glycidol	74	C3H6O2	000556-52-5	9





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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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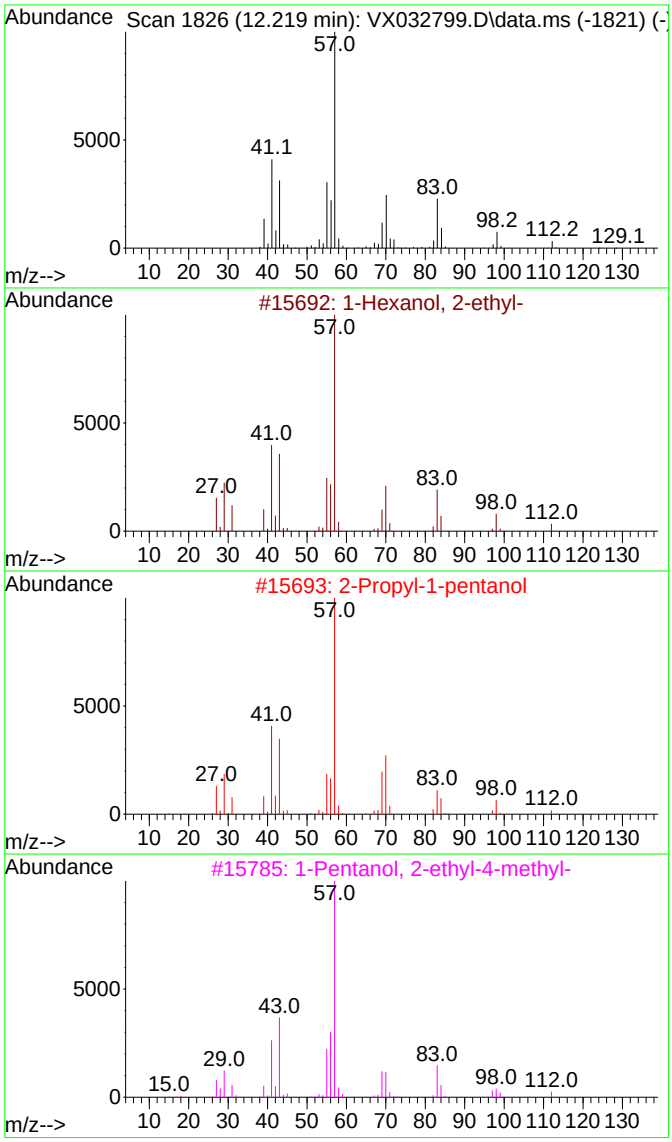
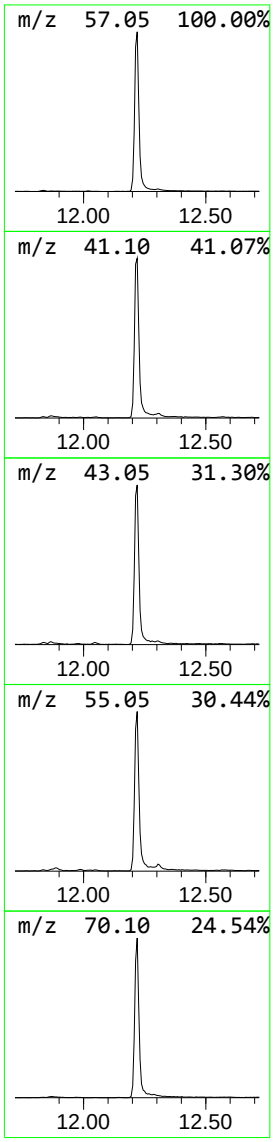
Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	119.80 ug/l	1062890	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
3	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
4	Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	53
5	1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	50





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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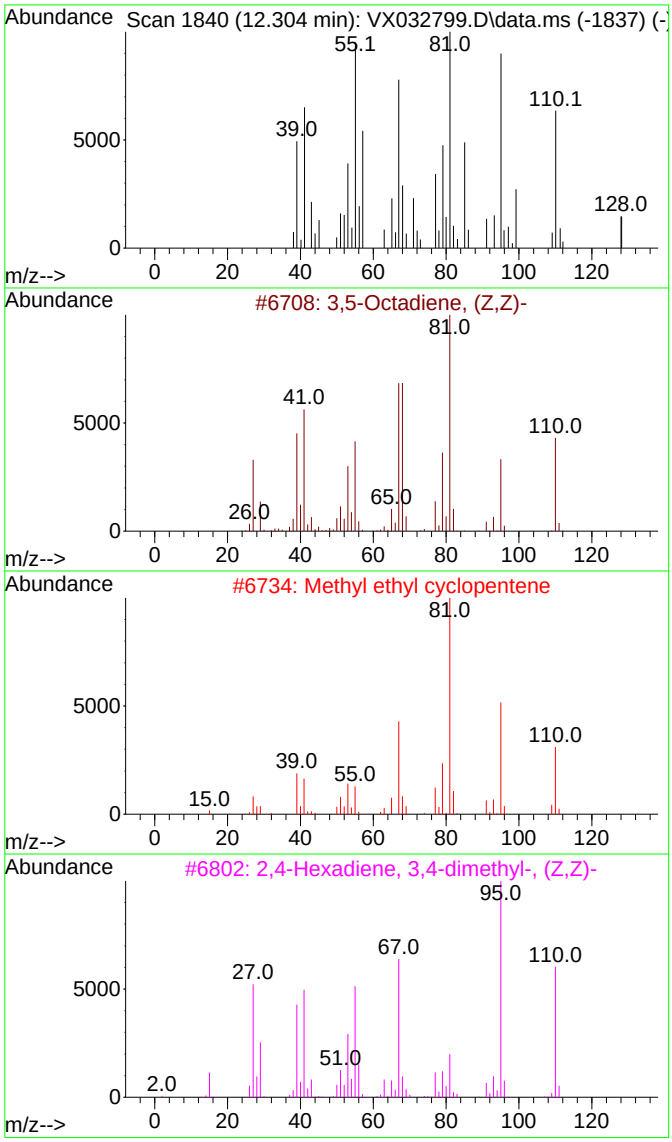
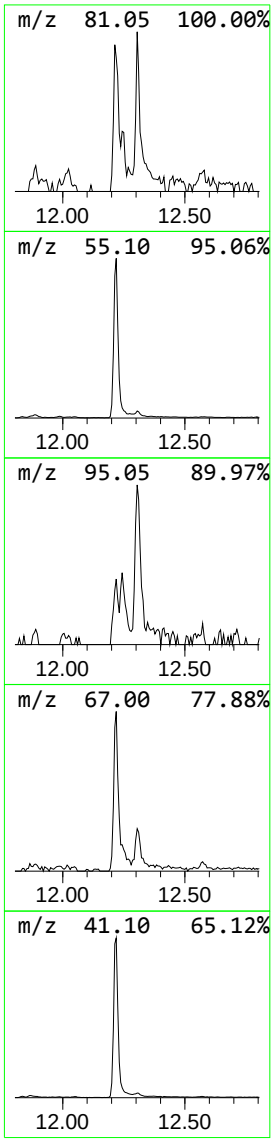
Peak Number 5 3,5-Octadiene, (Z,Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.304	6.00 ug/l	53266	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-Octadiene, (Z,Z)-	110	C8H14	007348-80-3	76
2	Methyl ethyl cyclopentene	110	C8H14	019780-56-4	70
3	2,4-Hexadiene, 3,4-dimethyl-, (Z...	110	C8H14	021293-01-6	64
4	2,4-Hexadiene, 3,4-dimethyl-, (E...	110	C8H14	002417-88-1	58
5	Cyclopropane, tetramethylmethylene-	110	C8H14	054376-39-5	58





Tentatively Identified Compound (LSC) summary

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TIC Library : C:\Database\NIST20.L
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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butanal	4.227	117.0	ug/l	664676	1	5.556	284151	50.0
1-Butanol	7.244	5.7	ug/l	42080	2	6.763	366347	50.0
Pentanal	7.574	12.3	ug/l	89968	2	6.763	366347	50.0
1-Hexanol, 2-et...	12.219	119.8	ug/l	1062890	4	12.024	443610	50.0
3,5-Octadiene, ...	12.304	6.0	ug/l	53266	4	12.024	443610	50.0